HIGH PERFORMANCE COMPUTING

AMD EPYC™ 7002 SERIES PROCESSORS AND GROMACS MOLECULAR DYNAMICS SIMULATION

AMD EPYC

AUGUST 2019

AMD EPYC for HPC

Utilizing the x86-architecture, and built on 7nm technology, the AMD EPYC™ 7002 Series processors bring together high core counts, large memory capacity, extreme memory bandwidth and massive I/O with the right ratios to enable exceptional HPC workload performance.

Standards Based Architecture

Continuing the AMD commitment to industry standards, AMD EPYC 7002 generation processors offer you a choice in x86 architecture. x86 compatibility means you can run your x86 based applications on AMD EPYC processors.

Exceptional Scalability

Scaling is critical to HPC applications. AMD EPYC 7002 Series processors provide high bandwidth between nodes with support for PCIe Gen 4 enabled network devices. Within node, take advantage of up to 64 cores per socket, including 8 memory channels utilizing speeds up to DDR4-3200[2]. Add incredible floating point and integer compute within each core and the AMD EPYC 7002 generation delivers exceptional performance and scalability for HPC.

Fully Tested and Validated

AMD's broad partner ecosystem and collaborative engineering provide tested and validated solutions that help lower your risk and total cost of ownership.

GROMACS

GROMACS is a high-performance molecular dynamics simulation solution. It simulates the Newtonian equations of motion for systems with hundreds to millions of particles.

AMD EPYC™ 7002 Processors: Architectural Innovations Deliver Exceptional Performance and Scalability

The high-performance computing (HPC) market has grown to a point where it is a critical component of new technology advancements in academia and a wide array of industries in both the public and private sectors. Scientific research, public health, climate modeling, as well as oil and gas exploration are just a few examples where HPC is the driving force behind new innovations and knowledge discovery.

7 nm	PCIe® Gen 4	DDR4 3200
64 Cores per socket	**128** PCIe® Gen 4 lanes per socket	**8** Memory channels per socket
World's first 7 nm x86 server CPU Highest available core count[1] to maximize parallelism	World's first PCIe® Gen 4 ready x86 server CPU[2] Doubles the bandwidth of the previous generation	World's first x86 architecture with DRR4 3200[2] Up to 4 TB of memory capacity per socket

The second generation of the AMD EPYC™ processor extends AMD innovation leadership for HPC. Built with leading-edge 7nm technology, the AMD EPYC™ SoC offers a consistent set of features across a range of choices from 8 to 64 cores, including 128 lanes of PCIe® Gen 4[2] and 8 memory channels with access to up to 4 TB of high-speed memory.

The AMD EPYC™ 7002 Series processor's innovative architecture translates to tremendous performance and scalability for HPC applications, offering you a choice in x86 architecture while optimizing total cost of ownership.

GROMACS and AMD EPYC: Power Without Compromise

GROMACS is a molecular dynamics package primarily designed for simulations of proteins, lipids, and nucleic acids. It supports all the usual algorithms expected from a modern molecular dynamics implementation.

GROMACS can be run in parallel in a multi-node environment using the standard MPI communication protocol. It is open-source software with the latest versions available under the GNU Lesser General Public License (LGPL). The code is mainly written in C and makes use of both MPI and OpenMP parallelism.

Many dynamics are involved with optimizing HPC applications. Core IPC is a critical factor in optimizing performance of GROMACS. AMD EPYC server

processors employing the "Zen2" microarchitecture helps ensure that you get the most out of your system, optimizing execution time overall utilization of your deployment.

High-Performance Compute (HPC) workloads require you to balance performance vs costs. AMD EPYC processors offer a consistent set of features across the product line, allowing users to optimize the number of cores required for their workloads without sacrificing features, memory channels, memory capacity, or I/O lanes. Whether you need 8 or 64 physical cores per socket, you will have access to 8 channels of memory per processor across all EPYC server processors

As workloads demand more processor cores, the communications between processor cores becomes critical to efficiently solving the complex problems faced by customers. As cluster sizes increase, the communication requirements between nodes rises quickly and can limit scaling at large node counts. AMD addresses this scaling limitation by partnering with leading network providers, such as Mellanox®, to offer high performance solutions based on PCIe Gen 4. PCIe Gen 4 allows incredible performance on Infiniband HDR 200Gb/s fabric when run on 2nd Generation EPYC processor-based clusters.

Performance Benchmarks and Testing

This document focuses on performance and scaling of the EPYC 7002 Series Processors. Testing was performed on a cluster of dual-socket EPYC 7742-based systems and dual-socket EPYC 7542-based systems.

Each EPYC™ 7742 processor has 64 cores with a base frequency of 2.25 GHz and a boost frequency of 3.4 GHz. Each EPYC™ 7542 processor has 32 cores with a base frequency of 2.9 GHz and boost of 3.4 GHz.

The compute nodes in the cluster are each populated with 1 DIMM per channel of 64-GB, dual-rank, DDR4-3200 DIMMs from Micron®, for a total of 1TB of memory per node.

A Mellanox® ConnectX-6 200 Gb/s HDR InfiniBand adapter, utilizing EPYC's support for PCIe Gen 4, is also populated on each EPYC-based system.

Single-node testing was performed across all platform configurations and multi-node scaling was tested on the EPYC 7742 processor.

Single-node testing was also performed on 2-socket platform using 1st Generation EPYC 7601 processors to show generational comparisons.

GROMACS Compilation

GROMACS version 2019.3, OpenMPI 4.0.0, and the AOCL 2.0 optimized version of FFTW were compiled from source on RHEL 7.6 using the AOCC 2.0 compiler. High level optimizations were set with -O3, the "Zen2" core architecture flag was set (-march=znver2), and AVX2 instructions were enabled (--enable-avx2). Various other compile options were also used and will be discussed in a planned future, more detailed, document,

GROMACS Benchmarks

The testing performed for this document was based on the lignocellulose3M_rf model that uses reaction field for electrostatics for Tier-0 systems. It is part of the Unified European Applications Benchmark Suite. More information on the benchmarks can be found here:

https://repository.prace-ri.eu/git/UEABS/ueabs/#gromacs

The benchmark can be downloaded directly from PRACE here:

http://www.prace-ri.eu/UEABS/GROMACS/1.2/GROMACS_TestCaseB.tar.gz

GROMACS: Single-node Performance

Figure 1 details the single-node performance of two-socket systems across each of the AMD EPYC processors. The 1st Gen EPYC 7601 and the 2nd Gen EPYC 7542 both have 32 cores per socket for a total of 64 cores per node. The 2nd Gen EPYC 7742 has 64 cores per socket for a total of 128 cores per node.

The performance shows a very strong generational improvement of ~68% between the EPYC 7601 and the EPYC 7542. Further, the results show that GROMACS can take advantage of the higher core count of the 2nd Gen EPYC 7742, with an impressive ~156% average performance boost over the 1st generation EPYC 7601.

Multi-threading was disabled in the cluster and the job was run in a pure MPI configuration during these tests. Planned follow-up testing will include Simultaneous Multi-Threading (SMT) enabled via BIOS and Hybrid MPI/OpenMP configurations.

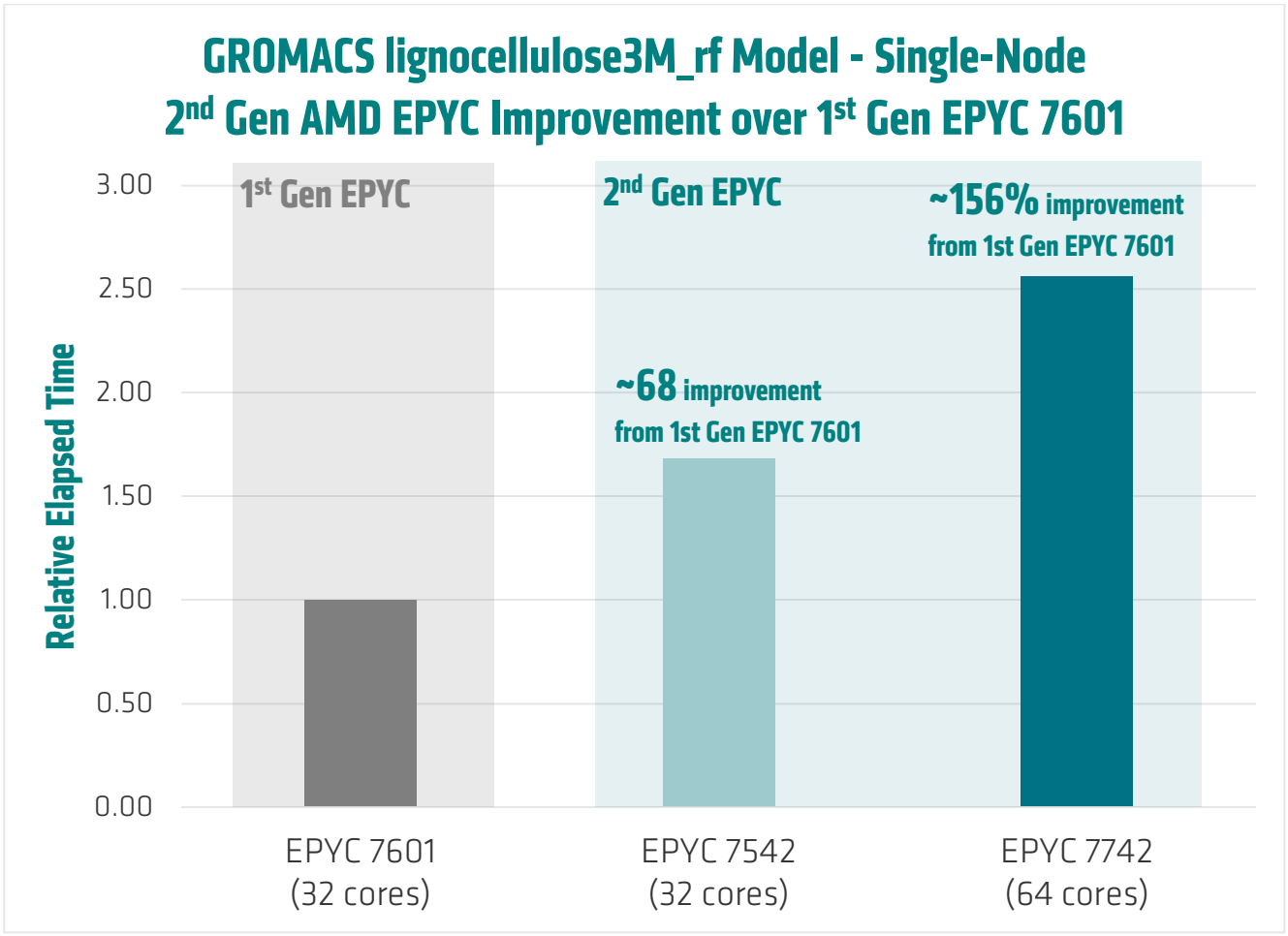

Figure 1

GROMACS: Multi-node Scaling

The lignocellulose3M_rf model from PRACE is used below to show how GROMACS scales on the 64-core EPYC 7742. Figure 2 shows very clean scaling through 8 nodes (1024 cores).

These results demonstrate the benefits of the balanced architecture of 2nd Generation EPYC processors. Fitting 128 cores into a single node without losing scalability, is accomplished by having very high memory bandwidth, bringing PCIe Gen 4 capabilities to the x86 market, and partnering with leading networking partners, such as Mellanox, to utilize the higher speed of PCIe Gen 4 with their InfiniBand HDR 200Gb/s fabric.

The density offered by having the incredible single-node performance of 128-core per node, combined with the scalability shown in Figure 2, and low power/performance enabled by 7nm technology, makes it easy to see why 2nd Generation EPYC processors is a great solution.

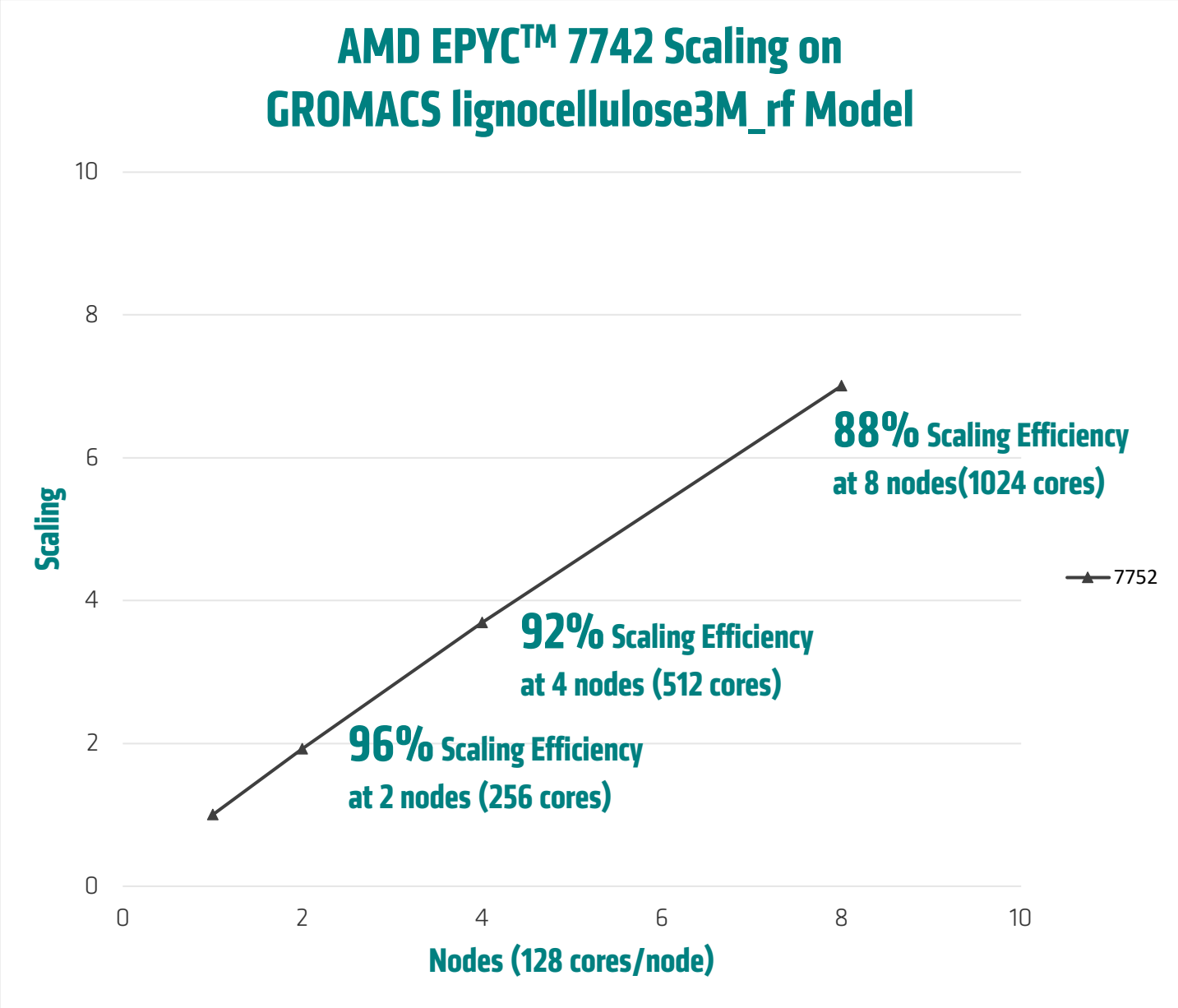

Figure 2

Summary

AMD engineers performed GROMACS benchmark testing on single nodes of two-socket systems, running 32-core and 64-core AMD 2nd Gen EPYC processors and showed incredible generational performance gains over the AMD 1st Gen EPYC 7601. The 64-core EPYC 7742 showed an ~156% performance increase and the 32-core EPYC 7542 showed an ~68% performance increase over the prior generation.

Scaling testing were then run on the lignocellulose3M_rf model from PRACE to show scaling of GROMACS on the EPYC 7742. Results show very good scaling of ~96%, ~92%, and ~88% at 2, 4, and 8 nodes, respectively.

Conclusion

Scale-out testing on the EPYC cluster shows impressive results running GROMACS. Pure performance was highest with the 64-core EPYC 7742. Per-core performance was highest with the 32-core EPYC 7542. Whether you need the dominating system level performance and density of the EPYC 7742 or the equally dominating per-core performance of the EPYC 7542, all products offer exceptional core IPC, and provide your organization a significant advantage. Customers can pick the optimal part based on their unique requirements.

AMD empowers the development of fast, accurate molecular dynamics simulations running on cost-effective clustered systems.

For more information about AMD's EPYC line of processors visit: https://www.amd.com/epyc

For more information about GROMACS visit: http://www.gromacs.org/

FOOTNOTES

1. Best-in-class based on industry-standard pin-based (LGA) X86 processors. NAP-166.
2. Some supported features and functionality of second-generation AMD EPYC™ processors (codenamed "Rome") require a BIOS update from your server manufacturer when used with a motherboard designed for the first-generation AMD EPYC 7000 series processor. A motherboard designed for "Rome" processors is required to enable all available functionality. ROM-06.

NOTE: Links to third party sites are provided for convenience and unless explicitly stated, AMD is not responsible for the contents of such linked sites and no endorsement is implied. GD-5